WHAT IS CLAIMED IS:

1. A method for modeling a system that includes a protein and a plurality of fragments in order to identify drug leads, the method comprising:

initiating a weighted Grand-Canonical Metropolis Monte Carlo simulation of the system;

subdividing the space of the simulation system with a grid, with x_i the centers of the grid cells;

initializing a numerical chemical potential field $B_{num} = B_0$ on the grid;

periodically sampling the Markov chain associated with the Metropolis Monte Carlo simulation, so as to compute the weighted number of sampled fragments per cell:

$$n_{B=0}(x_i) = \frac{1}{n_{\text{samples}}} \sum_{\text{samples}} \sum_{\text{frag j in cell i}} \exp\left[-B_{\text{num}}(Y_j)\right]$$

adapting the field $B_{num}(x)$ such that

$$B_{\text{num}}(x_i) = \log\left(\frac{n_{\text{target}}}{n_{B=0}}\right),$$

fixing the field $B_{num}(x)$ such that the Markov chain associated with the Metropolis Monte Carlo simulation equilibrates; and

outputting samples from the equilibrated Markov chain.

2. The method of claim 1, further comprising:

sampling the Markov chain periodically, with sufficiently long interspacing to ensure decorrelated states; and

obtaining positions, orientations, fragment-protein potential energies and statistical weights for all fragments at each state.

3. The method of claim 2, further comprising:

performing binding analysis of the system, based on the positions, orientations, fragment-protein potential energies, and statistical weights for all fragment states provided by the sampling.

4. The method of claim 3, wherein said performing step comprises:

i) making use of the properties of the Grand Canonical ensemble to estimate the binding affinity of the fragment for different regions of the protein surface by assigning a critical value B_c to each fragment-residue pair, using the positions, orientations, fragment-protein potential energies, and statistical weights for all fragment states provided by the sampling; and

ii) identifying potential binding sites on the protein based on the B_c values.

5. The method of claim 2, further comprising:

assembling the fragments into drug leads in the binding sites, based on binding affinity of the different fragments (B_c values), and on geometric proximity using rules by which organic fragments may bond together.

6. A computer program product comprising a computer usable medium having computer readable program code that enables a computer to model a system that comprises a protein and a plurality of fragments in order to identify drug leads, the computer program product comprising:

first computer readable program code that initiates a weighted Grand-Canonical Metropolis Monte Carlo simulation;

second computer readable program code that causes the computer to subdivide the space of the simulation system with a grid, with x_i the centers of the grid cells;

third computer readable program code that causes the computer to initialize a field $B_{num}(x_i) = B_0$;

fourth computer readable program code that causes the computer to compute the weighted number of sampled fragments per cell,

$$n_{B=0}(x_i) = \frac{1}{n_{\text{samples}}} \sum_{\text{samples}} \sum_{\text{frag j in cell i}} \exp[-B_{\text{num}}(Y_j)]$$

fifth computer readable program code that causes the computer to adapt the field $B_{num}(x)$ such that

$$B_{\text{num}}(\mathrm{x}_i) = \log\left(\frac{n_{\text{target}}}{n_{B=0}}\right),$$

sixth computer readable program code that causes the computer to keep the field $B_{num}(x)$ fixed, so that the Markov chain associated with the Metropolis Monte Carlo scheme can equilibrate; and

seventh computer readable program code that causes the computer to output samples from the equilibrated Markov chain.

7. The computer program product of claim 6, further comprising:

seventh computer readable program code that causes the computer to sample the Markhov chain periodically at successive decorrelated states; and

eighth computer readable program code that causes the computer to obtain positions, orientations, fragment-protein potential energies, and statistical weights for all fragments at each state.

8. The computer program product of claim 7, further comprising:

ninth computer readable program code that causes the computer to perform binding analysis based on the positions, orientations, and statistical weights for all fragments at each state.

9. The computer program product of claim 8, wherein said ninth computer readable program code comprises:

computer readable program code that causes the computer to assign a critical value B_c to each fragment-residue pair based on the positions, orientations, and statistical weights for all fragments at each state; and

computer readable program code that causes the computer to identify potential binding sites on the protein based on the B_c values.

10. The computer program product of claim 8, further comprising:

tenth computer readable program code that causes the computer to assemble the fragments into drug leads based on binding affinity of the different fragments (B_c values), and on geometric proximity using rules by which organic fragments may bond together.

11. A system for modeling a system that includes a protein and a plurality of fragments in order to identify drug leads, the system comprising:

A. means for initiating a weighted Grand-Canonical Metropolis Monte Carlo simulation of the system;

B. means for subdividing the space of the simulation system with a grid, with x_i the centers of the grid cells;

C. means for initializing a numerical chemical potential field $B_{num} = B_0$ on the grid;

D. means for computing the weighted number of sampled fragments per cell,

$$n_{B=0}(x_i) = \frac{1}{n_{\text{samples}}} \sum_{\text{samples}} \sum_{\text{frag j in cell i}} \exp\left[-B_{\text{num}}(Y_j)\right\}$$

E. means for adapting the field $B_{num}(x)$ such that

$$B_{\text{num}}(\mathrm{x}_i) = \log\left(\frac{n_{\text{target}}}{n_{B=0}}\right),$$

F. means for fixing the field $B_{num}(x)$ such that the associated Markhov chain equilibrates; and

G. means for outputting samples from an equilibrated Markov chain.